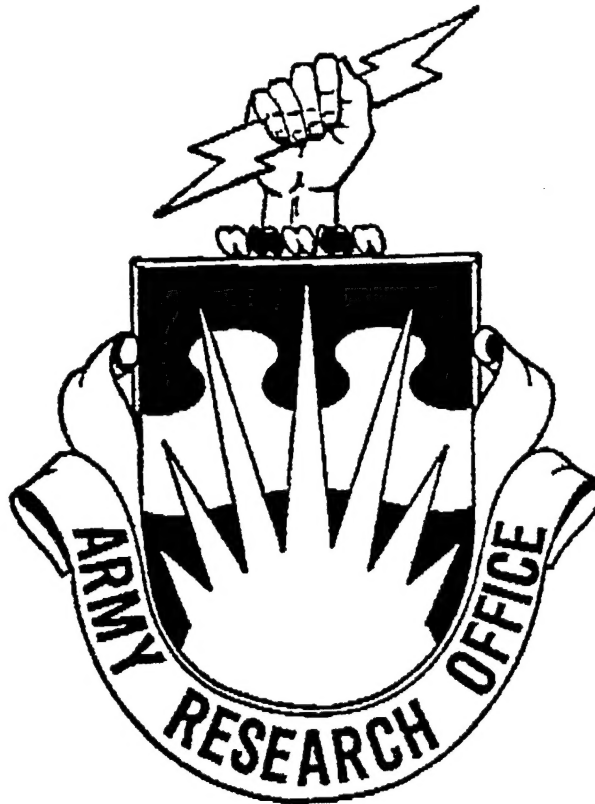


Final Report

New Concepts in Decontamination Workshop



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**October 5 – 7, 1995
Jackson Hole, Wyoming**

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Preface

Reginald P. Seiders
Army Research Office

A joint ARO/ERDEC Workshop on New Concepts in Decontamination was held on 5-7 October, 1995 in Jackson Hole, Wyoming. Excellent professional and efficient local support was provided by personnel from the Conferences and Institutes Office of the University of Wyoming. Participation in this workshop was by invitation only and was limited to less than 50 scientists. As you will see from this report, representatives from the three Services, Academia, and the National Labs at Oak Ridge, Los Alamos, and Lawrence Livermore participated in this meeting.

The motivation for this workshop was threefold: (1) the concern over the very low priority of decontamination research among the Joint Services Material Group's priority list of chemical and biological defense mission areas; (2) the recognition that it had been over seven years since the last workshop on this topic and the timeliness of bringing this research community together again; and (3) the recognition that there were still very difficult problems in decontamination which needed to be highlighted by the research community.

As can be seen from the agenda, the format of the workshop consisted of two full days of 30- to 40-minute oral technical presentations with a discussion and question period. These presentations were followed by another half-day session which began with brief Service-specific needs/problems in decontamination, and ended with group discussion of several specific decontamination topics, such as wide area decon and sensitive equipment decon.

It appeared that the workshop was an unqualified success in stimulating discussion among the participants. It should be noted that the DOE lab representatives were active participants in this workshop and they provided some fresh ideas and viewpoints which were most welcome. The results tallied in the overall workshop evaluation also showed that the participants were quite satisfied with the site and content of this workshop. Specific written comments on the workshop or on general decontamination research were invited, and several are included at the end of this report for the interested reader.

New Concepts in Decontamination Workshop Agenda

Wednesday, October 4

1900 - 2100 Registration — Motel Lobby

Thursday, October 5

0730 Continental Breakfast — Rimrock Room
0800 Registration — Motel Lobby
0845 Welcome and Administrative Details
0900 *Cleavable Surfactants in Decontamination*
David Jaeger, Department of Chemistry, University of Wyoming,
Laramie, WY
0940 *Combinatorial Catalysis*
Frederic Menger, Department of Chemistry, Emory University, Atlanta, GA
1020 - 1040 Break
1040 *Polyoxometallates in Decontamination*
Craig Hill, Department of Chemistry, Emory University, Atlanta, GA
1120 *Construction and Utilization of Functionalized Unimolecular Micelles*
George Newkome, Department of Chemistry, University of South Florida, Tampa, FL
1200 - 1330 Lunch (on your own)
1330 *Individual Decontamination: The Role of Physical Organic Chemistry*
Clifford A. Bunton, Department of Chemistry, University of California,
Santa Barbara, CA
1410 *Direct Oxidation by Persulfate*
John Cooper, Lawrence Livermore National Lab, Livermore, CA
1450 - 1520 Break
1520 *Surfactant-Based Decontamination Systems*
Raymond A. Mackay, Clarkson University, Potsdam, NY
1600 *Ozone Mitigation of Biological Warfare Agents*
Donald Pettit, Los Alamos National Lab, Los Alamos, NM
1640 *Decontamination Using Supercritical Carbon Dioxide*
Craig Taylor, Los Alamos National Lab, Los Alamos, NM
Dinner (on your own)
1930 Evening presentations (to be announced)

Friday, October 7

- 0745 Continental Breakfast — Rimrock Room
- 0820 *Cationic Colloids for Catalytic Decontamination*
Warren Ford, Department of Chemistry, Oklahoma State University, Stillwater, OK
- 0900 *Structure and Reactivity of Artificial Dinuclear Phosphoesterases*
Jik Chin, McGill University, Montréal
- 0940 *Decon and Demil with Carbonaceous Adsorbents*
Russell S. Drago, Department of Chemistry, University of Florida, Gainesville, FL
- 1020 - 1040 Break
- 1040 *Cleavages of Phosphonothioates, Phosphotriesters, and Phosphodiesteres; Studies of Azobenzene-lipid 'Photosomes'*
Robert A. Moss, Department of Chemistry, Bush Campus of Rutgers University, Piscataway, NJ
- 1120 *Plasma-Based Decontamination of Surfaces Using Singlet Metastable Oxygen*
Gary S. Selwyn, Los Alamos National Lab, Los Alamos, NM
- 1200 - 1330 Lunch (on your own)
- 1330 *Bacterial Enzymes for the Decontamination of Organophosphorus Nerve Agents*
Joseph J. DeFrank, Research and Technology Directorate, ERDEC,
Aberdeen Proving Ground, MD
- 1410 *Noncorrosive Quaternary Ammonium Complex Decontaminant*
Donald T. Cronic, Naval Surface and Weapons Center, Dahlgren, VA
- 1450 - 1520 Break
- 1520 *Biocatalytic Destruction of Chemical Weapons*
Alan Russell, Department of Chemical Engineering and Biotechnology,
University of Pittsburgh, Pittsburgh, PA
- 1600 *Applications of Polyethylene Glycol Chemistry in Decontamination*
J. Milton Harris, Department of Chemistry, University of Alabama, Huntsville, AL
- 1640 *Structure and Mechanism of Action for an Enzyme Capable of Hydrolyzing Organophosphate Nerve Agents*
Frank Raushel, Department of Chemistry, Texas A & M University,
College Station, TX
Dinner (on your own)

Saturday, October 7

- 0730 Continental Breakfast — Rimrock Room
- 0830 - 0900 *Nanoscale Metal Oxides as Destructive Adsorbents. New Surface Chemistry and Environmental Applications*
Kenneth Klabunde, Department of Chemistry, Kansas State University,
Manhattan, KS
- 0900 - 1200 Group Discussions: (rooms to be announced)
DOD Needs and Future Directions of Research in Decontamination

Abstracts

Jaeger, David A. (Department of Chemistry, University of Wyoming, Laramie, Wyoming)

Cleavable Surfactants in Decontamination

Two new cleavable double-chain surfactants with two head groups have been prepared, and their derived vesicles have been characterized by ¹HNMR, dynamic laser light scattering, differential scanning calorimetry, and gel filtration chromatography. One surfactant contains a ketal linking group and two carboxylate head groups. The other, based on Girard's reagent, contains a hydrazone linking group and quaternary ammonium and carboxylate head groups. The vesicles of each surfactant have the potential to simultaneously decontaminate and signal the presence of mustard as follows: (1) mustard, solubilized within a vesicle, reacts to form the corresponding episulfonium ion, which is captured by a carboxylate head group; (2) with this alkylation of the head group by mustard, which effects decontamination, the vesicle should become more permeable or, ideally, undergo a change to micelle morphology; (3) in either event, a water-soluble signaling agent would be released from the vesicle interior. Trial reactions to date with two mustard simulants (methyl 2-chloroethyl sulfide and phenyl 2-chloroethyl sulfide) have been performed with the second of the two surfactants described above. We have not yet demonstrated alkylation of the carboxylate head group. The potential for simultaneous decontamination and signaling of mustard remains intact however. It may be necessary to study alternate surfactants systems with nucleophiles stronger than carboxylate.

Menger, Frederic (Department of Chemistry, Emory University, Atlanta, Georgia)

Combinatorial Catalysis — Abstract not available.

Hill, Craig (Department of Chemistry, Emory University, Atlanta, Georgia)

Polyoxometallates in Decontamination — Abstract not available.

Newkome, George R. (Center for Molecular Design and Recognition, University of South Florida, Tampa, Florida)

Construction and Utilization of Functionalized Unimolecular Micelles

Cascade polymeric architectures possessing internal functionalities have been employed for the preparation of Metallomicellane™ derivatives. Heterocascade synthesis employing different building blocks in order to ensure metal ligand connectivity and stability will be reported. The relationship of the interior cascade reactivity to the macromolecular internal "void regions" has been probed and evaluated by molecular encapsulation of guest molecules. Preliminary catalytic studies will be considered.

Bunton, Clifford A. (Department of Chemistry, University of California, Santa Barbara, California)

Individual Decontamination. The Role of Physical Organic Chemistry

Chemical methods of individual decontamination require mild reagents. Oxidants will destroy Mustard and VX, nucleophiles react readily with G agents and VX is also destroyed by various alpha effect nucleophiles. Peroxy acids, e.g., magnesium peroxyphthalate, are potentially useful oxidants, and at pH>8 they form peroxyanions which are effective as nucleophiles. Organic solvents or solubilizing agents, e.g., association colloids such as micelles or microemulsions, will probably be needed to handle very hydrophobic or viscous thickened agents and their effects on reaction rates have to be considered. Rates of nucleophilic attack on phosphorus (V) esters initially decrease on addition of organic solvents to water, go through minima, and increase sharply in the drier solvents. Rates of oxidation by peroxyacids decrease significantly with decreasing water content of the solvent. Surfactant-derived micelles and microemulsions can increase rates by incorporating both reactants and concentrating them at the microdroplet surfaces. The overall rate constants therefore depend on transfer equilibria between water and the colloids, e.g., micelles, and local rate constants in water and at the micellar surface. For reactions of anionic nucleophiles rate constants in these two regions are similar, but oxidations by peroxyacids are relatively slow at micellar surfaces. With constant [reagent] overall rate constants go through maxima with increasing [surfactant], so if high [surfactant] is used to solubilize agents rate enhancements will be small or nonexistent. Rate enhancements also decrease with increasing concentration of reagent, e.g., nucleophile, which must be considered in extrapolating from laboratory to field conditions. Some of these "dilution" problems are reduced by using functionalized surfactants.

Cooper, John (Lawrence Livermore Lab, Livermore, California)

Direct Oxidation by Persulfate — Abstract not available.

Mackay, Raymond A. (Center for Advanced Materials Processing, Clarkson University, Potsdam, New York)

Surfactant-Based Decontamination Systems

There are a number of different needs for decontamination of chemical agents ranging from field expedients to installation cleanups. For each of these scenarios, the time scale and logistics of the operation can vary widely. In each case, however, two generic components are required: a means of agent collection and a method of agent destruction. The focus of this presentation is on the use of surfactant-based liquid media for the collection of the agent, with or without inclusion of a reagent system. A number of general approaches will be discussed, along with a few specific examples.

Pettit, Donald (Los Alamos National Laboratory, Los Alamos, New Mexico)

Ozone Mitigation of Biological Warfare Agents

We propose to use ozone dispersed as a dilute gas or as an aqueous solution to kill biological pathogens released into the atmosphere or spread on solid surfaces. Applications are especially suited to the release in confined spaces, buildings, tunnels, or in the decontamination of the exposed interiors of airplanes and vehicles. Collateral damage could be reduced when a terrorist device is deactivated or when a production facility is destroyed by suppressing the release of viable pathogen. Ozone in air is highly toxic to single-celled organisms at concentrations less than 1000 ppm, yielding kill times of the order of minutes. *Bacillus anthracis* spores in aqueous solution are killed in 15 minutes at 10 ppm and *Staphylococcus aureus* are killed in less than 10 seconds at 8 ppm. Ozone self-decomposes within about 30 minutes into oxygen and the oxidized by-products, mainly carbon dioxide and water, thus leaving no toxic residue. At 1000 ppm, fatal human exposures are of the order of 30 to 60 minutes which gives ample time for evacuation, thus, risk to human life can be minimized. Ozone in gas phase will permeate into cracks and nooks of sight cul-de-sacs. Ozone is a powerful oxidizer and may prove effective against the destruction of chemical warfare agents as well. Ozone as the stable cryogenic liquid, OZ-OX, is 20 wt% ozone in solution with liquid oxygen (at 90 K) with a bulk density of 1.23 g/cm³. One gallon of OZ-OX will disinfect 1400 m³, thus a small initial volume will treat a large infected zone. OZ-OX allows for effective delivery and sudden dispersal into infected areas via air drop or manual point placement. Due to the cryogenic nature of OZ-OX, it can only be stored for a few days and will need to be made at a forward-positioned facility near the point of intended use. Ozone generated on demand (thus by-passing storage issues) from a field portable trailer would allow decontamination of buildings, airplanes, vehicles, and field gear where the time-critical dispersal of OZ-OX is not needed. Ozone as a gas in air works well for the decontamination of interior surfaces where it could permeate into cracks and behind control panels. Exterior surfaces are best hosed down with aqueous ozone solutions. Both could be made from one trailer unit. Ozone in gas phase allows for dry decontamination in water-scarce regions.

Taylor, Craig (Supercritical Fluids Experimental Facility, Chemical Science and Technology Division, Los Alamos National Laboratory, Los Alamos, New Mexico)

Decontamination Using Supercritical Carbon Dioxide

Because of their high diffusivities, low viscosities, and temperature-pressure dependence of solvent strengths, supercritical fluids are attractive solvents for cleaning and removal of hazardous organic compounds from a wide variety of materials. These unique properties of supercritical fluids allow for solvent penetration into small, intricate structures. It is therefore possible to clean and decontaminate many items ranging from very small components containing small internal parts to large bulk machinery without requiring disassembly. In addition, such an application using a supercritical fluid such as carbon dioxide (CO₂) would be safer and faster as well as environmentally benign and less expensive than similar processes using chemical treatment methods. These properties render using CO₂ potentially advantageous for decontamination processing. It is possible to decontaminate, disinfect, destroy, sterilize, and/or remove bacteria, spores, viruses, and other living organisms from inanimate objects without the environmentally or physically deteriorative effects associated with thermal and chemical methods using supercritical (dense phase pressurized) fluids. In the supercritical state, CO₂ inactivates microorganisms. Carbon dioxide is able to penetrate the cell membrane and extract vital lipids from the cell, denature or inactivate vital proteins and enzymes, or physically disrupt the cell, thus terminating organism viability. Through these mechanisms, disinfection, decontamination, and/or demilitarization of biologically contaminated materials is possible. Supercritical fluid processing can also be applied to chemical contamination. Typical methods employed for chemical decontamination involve the use of liquid solvents for washing, dissolution, and extraction of the contaminants. Solvent washing or extraction using supercritical fluids offers the previously mentioned advantages over conventional solvent extraction as well as the minimization of organic liquid waste and their reduction in exposure of personnel to toxic organic solvent vapors. Using supercritical CO₂ containing a suitable complexing agent, radioactive contamination can be effectively removed from surfaces, collected, and disposed. Finally, from a practical standpoint, decontaminated equipment is removed from the cleaning chamber clean and dry, ready for immediate use. For these reasons, decontamination of equipment and surfaces using this approach has several potential advantages over current methods.

Ford, Warren T. (Department of Chemistry, Oklahoma State University, Stillwater, Oklahoma)

Cationic Colloids for Catalytic Decontamination

Polystyrene latexes, containing quaternary ammonium ions within the gel phase of the colloidal particles, speed chemical reactions in aqueous media. The rates of decarboxylation of 6-nitrobenzoxazole-2-carboxylate and of IBA-catalyzed hydrolysis of *p*-nitrophenyl diphenyl phosphate are 10,500 and 6,000 times faster respectively in the presence than in the absence of 0.5 or 0.2 mg/mL of a latex containing polymer-bound benzyltributylammonium ions. The mechanism of action of an ion exchange latex is similar to that of a micelle, and the kinetics are analyzed by an ion exchange mechanism. Partitioning of organic compounds into the latex and exchange of anions from water provide high local concentrations of ionic and organic reactants in the polymer phase, and account for most of the rate enhancements. In contrast, hydrolyses of the VX simulant Tetriso and of diisopropyl fluorophosphate in basic media containing no nucleophilic catalyst showed no rate acceleration by latex (results of J. Walker and F. Hoskin, Natick RD & E Center), which we attribute to low solubility of these simulants in polystyrene latexes. Future research on colloidal media for catalytic decontamination will focus on acrylic latexes to dissolve aliphatic agents, latexes surface stabilized with poly(ethylene oxide) to make them colloidal stable in media of high electrolyte concentration such as sea water, polyampholyte latexes that swell with increasing electrolyte concentrations, and dendritic polymers modified at interior sites with quaternary ammonium ions.

Seog Seo, Jin, Bryan Takasaki, Daphne Wahnnon, Nick Williams, Mary Jane Young, and Jik Chin,
(Department of Chemistry, McGill University, Montréal, Canada)

Structure and Reactivity of Artificial Dinuclear Phosphoesterases

In nature there are many enzymes that catalyze the hydrolysis of phosphate esters as well as those that catalyze the synthesis of phosphate esters that are activated by two or more metal ions. They include DNA polymerase,^[1] 3', 5'-exonuclease,^[1] RNase H,^[2] P1 nuclease,^[3] alkaline phosphatase,^[4] and phospholipase C.^[5] Tetrahymena ribozyme is also thought to be activated by at least two metal ions.^[6] Over the years, numerous interesting dinuclear metal complexes have been synthesized, their crystal structures determined and their spectroscopic properties analyzed.^[7] We have recently been interested in developing dinuclear metal complexes that efficiently hydrolyze phosphate esters^[8] based on what we have learned about the reactivity of mononuclear metal complexes.^[9] Dinuclear Co(III) (Figure 1), Cu(II), Zn(II), and Ln(III) complexes that possess unusual reactivity for hydrolyzing phosphate esters including nucleic acids will be presented.

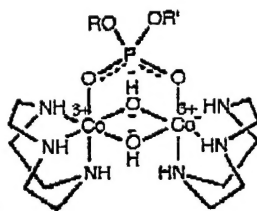


Figure 1. Dinuclear Co(III) complex with a bridging phosphate diester.

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Drago, Russell S., J. Michael McGilvray, Alfredo Mateus, and Kenneth Lo (Department of Chemistry, University of Florida, Gainesville, Florida)

Decon and Demil with Carbonaceous Adsorbents

Carbonaceous adsorbents have a high affinity for mustard and other agents. This property has led to the use of these materials in the Basic Soldier Skills Decon Kit. A more widespread application of these materials would remove agents in decon and demil applications and contain them in the pores of the solid. In the ideal situation, the agents would be decomposed catalytically on standing. The research to be presented focuses on two aspects of the problem. (1) To obtain a fundamental understanding of the adsorption process. This understanding would lead to the characterization and design of better adsorbents. (2) To find catalysts that will oxidize agents contained in the pores of the carbon. This objective would permanently dispose of the agent and would permit regeneration of the adsorbent or make it safe for disposal. Progress and future research targets in both areas will be presented.

Moss, Robert A. (Department of Chemistry, Rutgers University, New Brunswick, New Jersey)

Cleavages of Phosphonothioates, Phosphotriesters, and Phosphodiesteres; Studies of Azobenzene-lipid 'Photosomes'

This presentation will consist of four topical sections: (1) The use of micellar iodosobenzoate/iodoxybenzoate to cleave phosphonothioate model substrates (VX simulants); (2) The comparative reactivities of various *p*-nitrophenyl phosphotriester substrates in cleavage reactions with micellar iodosobenzoate and iodosonaphthoate reagents; (3) The cleavage of micellar and liposomal phosphodiester substrates by lanthanide ions; and (4) Some properties of photoresponsive liposomes ('photosomes') constructed from cationic lipids bearing an azobenzene-containing chain.

Selwyn, Gary S. (Plasma Physics, Los Alamos National Laboratory, Los Alamos, New Mexico)

Plasma-Based Decontamination of Surfaces Using Singlet Metastable Oxygen

Plasmas are a rich source of energy-excited and chemically-reactive fragments. Electron impact excitation of stable feedgas species results in chemical bond dissociation and high energy activation of ions and neutrals. Plasmas are also a safe and efficient means of generating short-lived reactive fragments. This is especially attractive since alternative, purely chemical approaches would otherwise likely involve highly toxic or hazardous feed stock or persistent effluent. This capability has been extensively utilized by the semiconductor industry for etching and deposition processes. We propose to extend this technology for application in surface decontamination for neutralization of chemical and biological warfare agents. We propose to develop a transportable, atmospheric-pressure plasma source to generate chemically-reactive effluent for neutralization of chemical and biological warfare agents. This approach builds upon the impressive and highly developed technology that has been developed by the semiconductor industry for plasma processing of their products. Our plasma source generates a unique and highly cytotoxic oxidant: $O_2(^1D_g)$. This reactant has 0.97 eV of internal energy, yet is derived from a feedgas that is incredibly safe, simple, and plentiful: oxygen or air and water. The advantage of this approach is that the decon unit is portable (requires only KW of electrical input), limitless (operates on air and water), is not size-limited (no decon chamber needed), it is safe to workers and the environment (reactive products harmlessly decay in less than 0.2 seconds), is "dry," and can decontaminate surfaces including clothes, electronics, munitions, vehicles, or breathing air fed into tanks, planes or bunkers without the need for specialized vacuum equipment. Equally important, the plasma effluent has potential for killing bacteria and viruses used as biological warfare agents and also may be used to neutralize chemical warfare agents. Unlike conventional decontamination methods involving solvents or bleach, the proposed plasma decon method does not corrode metal surfaces and paint and does not destroy wiring, electronics, or most plastics. This paper study will detail the practicality of producing an atmospheric-pressure plasma source of singlet metastable oxygen, the reactivity of this agent to chemical compounds and the toxicity of the oxygen metastable to bacteria and viruses, a role that has been widely studied in medical research for over 25 years.

Cheng, Tu-chen, Joseph J. DeFrank, and Amy B. Hamilton (U.S. Army Edgewood Research, Development and Engineering Center, Aberdeen Proving Ground, Maryland); and Lin Liu and David Anderson (ChemGen Corporation, Gaithersburg, Maryland)

Bacterial Enzymes for the Decontamination of Organophosphorus Nerve Agents

Continuing studies at the Edgewood Research, Development and Engineering Center (ERDEC) have demonstrated the potential efficacy of using enzymes from strains of *Alteromonas* and other halophilic bacteria for the decontamination of nerve agents such as soman, sarin, and tabun. Several of these bacterial Organophosphorus Acid (OPA) Anhydrolases have been purified and characterized. The genes for several of these enzymes have recently been cloned and sequenced. Based on their DNA/amino acid sequence it has been determined that these bacterial OPA Anhydrolases are actually dipeptidases and apparently have little or no role in phosphorus metabolism. Characterization of their dipeptidase activity is currently underway. As a means of disseminating an enzyme-based decontaminant, the use of foams (fire-fighting and others) is being examined. Foam-based systems would provide the contact time necessary for the enzymes to act and could also serve to assist in the solubilization of the agents. Preliminary results indicate that the enzymes will function quite well in solutions of the foam components.

Cronce, Donald T. (Naval Surface Warfare Center, Dahlgren Division, Dahlgren, Virginia)

Noncorrosive Quaternary Ammonium Complex Decontaminant

A need exists for a chemical warfare agent (CWA) decontamination solution which is noncorrosive, nontoxic, nonflammable, and environmentally safe. This decontamination solution should be effective against all agents, be stable in storage, be usable on all surfaces and reduce the logistical burdens associated with the current decontaminants. Prototype formulations have been developed, using quaternary ammonium complexes (QAC) and other components not listed as being corrosive, toxic, or flammable. The original formulation was composed of the QAC solvated in a glycol solvent and contained a buffer and a corrosion inhibitor. This formulation was evaluated for its effectiveness in neutralizing select CWA (HD, GD, VX); although the formulation appeared to react with the CWA, the assumed reactions were either slow, incomplete, or inefficient in detoxifying the agents. A modified formulation was developed after the initial CWA tests. The glycol was replaced by a small amount of water and the amount of corrosion inhibitor (an amino alcohol) was increased. The modified formulation was substantially more effective in neutralizing the CWA than the original formulation. Results of tests of the two prototype formulations are presented and discussed.

Russell, Alan J. (Department of Chemical Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania)

Biocatalytic Destruction of Chemical Weapons

Over 30 million kilograms of organophosphorus esters are used annually in the United States. The usefulness of these compounds is due to their inhibition of acetylcholinesterase in insects. This is also the primary cause of toxicity in nontarget organisms, including humans. Indeed, organophosphate esters of appropriate structure are so toxic that they are the most commonly manufactured nerve gas agents. Exposure to high levels of organophosphorus compounds has both acute and serious health consequences, and also results in delayed chronic cholinergic and neurological toxicity. Phosphotriesterase has been shown to be an effective catalyst for the continuous decontamination of a nerve agent in a continuous gas phase reactor. Very small quantities of the enzyme are sufficient to enable detoxification of low concentrations of the nerve agent for extended periods of time. In the case where the nerve agent is at high concentrations (a liquid) the enzyme has also been shown to be active in biphasic mixtures of a solvent with water. The activity and specificity of the enzyme in both environments (continuous gas phase and biphasic mixture) obey classical models of enzyme kinetics. The application of the enzyme in these systems depends on efficient immobilization of the enzyme. The generation of highly stable polyurethane-protein air filters which simultaneously remove and degrade a variety of chemical weapons will be discussed. An experimental demonstration of the activity and stability of such protein polymers will also be performed.

Harris, J. Milton (Department of Chemistry, University of Alabama in Huntsville, Huntsville, Alabama)

Applications of Polyethylene Glycol Chemistry in Decontamination

My research group has long had an interest in biomedical and biotechnical applications of hydrophilic, biocompatible polymers such as polyethylene glycol (or "PEG"). Four prime applications of PEG chemistry are: (1) covalent attachment to proteins to extend blood circulation times; (2) covalent attachment to enzymes to impart organic solubility; (3) surface coatings to prevent fouling in a biological environment; and (4) formation of hydrogels for wound covering, cell encapsulation, drug delivery, and enzyme immobilization. In the first part of this lecture I will present some recent studies on preparation and characterization of new PEG derivatives for protein modification. These new derivatives exhibit chemical selectivity and reactivity differences that are of practical advantage in protein attachment. Kinetic examination of these derivatives reveals surprising differences in hydrolytic reactivity. In the second part of my lecture I will describe the use of these new PEG derivatives in preparing biodegradable hydrogels, both with and without tethered enzymes. Applications to decontamination will be described.

Raushel, Frank M. (Department of Chemistry, Texas A & M University)

Structure and Mechanism of Action for an Enzyme Capable of Hydrolyzing Organophosphate Nerve Agents

The phosphotriesterase from *Pseudomonas diminuta* catalyzes the hydrolysis of organophosphate insecticides and military nerve agents. The active site of this protein has been probed by kinetic investigations, structure-reactivity relationships, NMR, EPR, site-directed mutagenesis and X-ray crystallography. It has been found that a coupled binuclear metal center is critical for the catalytic activity of this protein. The two divalent cations are ligated to the protein by four histidine residues, one aspartate, and are bridged by a carbamate functional group formed from the reaction of carbon dioxide with the side chain of lys-169. It is proposed that one metal functions to activate the hydrolytic water molecule while the other serves to polarize the phosphoryl oxygen bond.

Klabunde, K. J., D. G. Park, J. V. Stark, O. Koper, S. Decker, Y. Jiang, and L. Lagadic (Department of Chemistry, Kansas State University, Manhattan, Kansas)

Nanoscale Metal Oxides as Destructive Adsorbents. New Surface Chemistry and Environmental Applications

An aerogel procedure combined with hypercritical drying has yielded magnesium oxide and calcium oxide in ultrahigh surface-area forms. These nanoparticles of MgO and CaO possess intrinsically higher surface reactivities, and serve as destructive adsorbents for a variety of toxic substances, including organophosphorus compounds, and chlorocarbons. They also serve to adsorb large amounts of gases very strongly, such as CO₂, SO₂, SO₃, and HX. A second generation of even more effective destructive adsorbents has been prepared by depositing a monolayer of transition metal oxide on the MgO or CaO nanoparticles, for example [Fe₂O₃]MgO, [NiO]CaO, [ZnO]MgO, and others. As a test reaction [FeCl₃]MgCl₂ + CO₂ was employed. This gas-solid reaction was facilitated and enhanced by two things: (1) unusual morphology of nanoscale MgO, probably because of exposure of {111} crystal faces and high concentrations of edge sites and defect sites, and (2) the presence of the thin layer of Fe₂O₃ (or other transition metal oxide), which allows a catalytic O²/Cl⁻ solid state ion/ion exchange to take place. The reaction proceeded to almost stoichiometric proportions when Fe₂O₃ was present, which indicates that the surface Fe₂O₃-FeCl₃ layer is mobile and dynamic, allowing continual O²/Cl⁻ exchange deeper into the nanoparticle. Morphological studies were aided by Atomic Force Microscopy experiments, which will also be discussed.

Workshop Summary Discussion

Reginald P. Seiders
Army Research Office

It was clear from the comments of the Service representatives that there are still critical issues in decontamination which need to be addressed. These issues range from the corrosiveness of currently fielded decontaminants such as DS-2 and STB, to the need for wide area decontamination for fixed sites such as ports and air bases. Furthermore, there is no decontaminant available at all for electronic equipment, except perhaps for hot air or natural weathering. Some of these issues are addressed below, and where appropriate, specific research or technology from the workshop is identified as a possible solution to the problem.

Wide Area Decontamination of Fixed Sites

Contamination of large areas such as seaports or air bases could be a show stopper. The Air Force is therefore appropriately interested in large scale decontamination. The Air Force may be more sensitive to casualties than the Army since the loss of even 5% of personnel from agent exposure could shut down an air base. We may want to reconsider hot air from jet engines for decontamination, and there is also the possibility of nondevelopmental items from the agriculture industry for decontaminant dissemination (e.g., sprayers and dusters). Use of aircraft deicing equipment and AFFF foam have also been suggested as having some merit in a decontamination scenario.

At this workshop several approaches to wide area decontamination were tentatively identified. Use of a mixture of phosphorus ester (and thioester)-hydrolyzing enzymes is conceivable, as has been suggested by DeFrank of ERDEC, but mustard would still be a problem because there is no enzyme to destroy mustard. The enzymes might be used as a free flowing powder, an aqueous solution probably with some detergent, or they might be incorporated into the AFFF foam. An added benefit of the foam would be that it would effectively remove the vapor hazard from any contamination. A second technique for large scale decon could be the use of sorbents such as polymer beads or latexes such as those studied by Ford at Oklahoma State, or activated charcoal such as that studied by Drago at the University of Florida. Preferably the sorbents would be modified with some reagent which would destroy the agent contaminant once it was trapped in the sorbent. The polyoxometallates studied by Hill at Emory show promise in this area, as do the iodosobenzoates made by Moss at Rutgers. Additionally, the very high surface area metal oxides studied by Klabunde at Kansas State could have utility if they are found to be reactive at ambient conditions. But Klabunde has actually advocated a more low-tech solution, and that would be simple agricultural limestone. It is cheap, readily available, and safe to use over wide areas. The alkaline properties of lime would ensure that it would react with the contaminants, but the rates and extent of reaction will need more study. A final method of wide area decon would be the use of surfactant-based formulations like the bleach-based microemulsion that was developed by Menger at Emory. At these large fixed sites, there would be minimal logistical difficulties with mixing and dispensing such a decontaminant. It has been shown to be rapid and effective, and is in fact being used by an agrochemicals company to clean-up pesticide spills.

Electronic Equipment Decontamination

It is a well recognized fact that the current decontaminants STB and DS-2 cannot be used on sensitive electronic equipment. The aqueous STB slurry would be very corrosive to the wiring and other metal parts of

the device, while the organic solvent qualities of DS-2 will adversely affect plastics, polymers and protective organic coatings. For the Air Force, avionics decontamination remains a technically challenging problem because of equipment sensitivity and inability to replace avionics as readily as other aircraft modules because of cost.

There were three presentations at the workshop by scientists from Los Alamos National Lab (see abstracts from Pettit, Taylor, and Selwyn) that were considered most relevant to electronic equipment decontamination. The first of these, gaseous ozone, should work well for decontamination of interiors and electronics modules, where it can penetrate into cracks and behind instrument panels. Ozone self-decomposes within about 30 minutes into oxygen and oxidized by-products, mainly carbon dioxide and water, thus leaving no toxic residue. As noted in the abstract, ozone should also be very effective against single-celled biological organisms. There have been studies of the reaction of ozone with chemical warfare agents, but this area should be studied further. (See for example Snelson, A.; Clark, D.; and Brabets, R.; Fluorocarbon/ozone + UV Decontamination System, in the Proceedings of the U.S. Army Chemical Research Development and Engineering Center Scientific Conference on Chemical Defense Research, November 1986, Volume 1, AD-B113 947, p33.)

The second method is supercritical carbon dioxide which is being developed at LANL as a small system to replace commercial dry-cleaning systems. (See Taylor's abstract.) This system should have promise for cleaning small electronics units (once compatibility issues are worked out). Of course because the supercritical system is at high pressure, many devices would have to be excluded. This system should also be useful for cleaning small items of a soldier's personal gear, and even the uniform in a laundry type facility. The supercritical carbon dioxide would function mainly as an extraction system, so that it would probably be necessary to have some type of reactant system to destroy the agent once it was removed. Many of the experimental decontaminants such as enzymes, oxidants, sorbents or hydrolysis catalysts could be considered for the role of reactant. This area could be a fruitful R&D topic if given suitable funding.

The third technique (see Selwyn's abstract) is more speculative because less experimental work has been done, however the plasma which contains singlet oxygen and reactive hydroxyl radicals should be very reactive with a wide array of organic compounds. A considerable experimental program is needed to confirm this however. It should be pointed out that a reactive plasma would also have the potential for killing bacteria and viruses which might be used in biological warfare. Also, unlike conventional decontamination employing solvents or bleach, this plasma method would not corrode metal surfaces or paint, and would not destroy wiring, electronics or most plastics.

Interior Decontamination

This is rather an unclear category because better definitions are needed for the types of interiors that are being considered. The method of decontamination could well depend on what was contained in that enclosed area. For example, the methods available for cleaning a helicopter cockpit are likely to be much more restrictive than those for cleaning the cargo area of a C-130 aircraft. Nevertheless, some of the research presented at the workshop could be recommended for interior decontamination. The ozone and plasma systems discussed above could be used in enclosed spaces. Indeed, if the space could be sealed off fairly tightly then the ozone could act as an effective "fumigant" of chemical and biological warfare agents, although R&D is needed to confirm and optimize this methodology. Sorbents such as metal oxides or polymers could also be used in some interior scenarios, and the enzyme "sponge" developed by Russell at Pittsburgh could

also be useful in cases where the contamination was confined to a relatively small surface.

The "holy grail" of decontamination science is the self-decontaminating surface or coating, and there is a system now available which nearly meets that description. Japanese scientists have been able to coat tiles, walls, and even some fabrics with a thin layer of titanium dioxide. This material is a well-known photocatalyst which, in the presence of oxygen and water will produce very reactive hydroxyl radicals on its surface when irradiated with UV light. These radicals will attack and destroy most organic compounds. The discovery that the Japanese have made is to show that there is enough residual UV light from ordinary fluorescent lights to activate the photocatalyst (on the tiled walls) and destroy noxious odors and chemicals in the room. It is not hard to imagine a similar coating on the interior surfaces of structures which would deactivate low levels of chemical agent vapor which has diffused to the coated surfaces. The natural fluorescent lighting which is used in most structures and buildings would be sufficient to activate the catalyst. This proposed system should definitely be investigated for use by the military as a passive chemical protection methodology.

Summary of Technical Issues

Some of the problems in decontamination were presented quite clearly by Prof. Bunton of the University of California at Santa Barbara. He reminded us that CW agent reactivity varies significantly. Some of the best detoxification reactions for one agent may be very poor for another. For example, HD hydrolyzes poorly but can be oxidized effectively while G-agents are readily detoxified by hydrolysis but do not react with many oxidants. Thus finding or developing decontaminants which are effective against the entire range of CW agents presents a serious challenge.

Decontamination efficiency of a liquid decontaminant is controlled by the rate of dissolution of agents into the decontaminant. The ability of surfactants to enhance solubilization of incompatible materials is a major reason that micelles and microemulsions have been investigated for decontamination formulations for a number of years. In the absence of surfactants, solvents of low polarity are required in the liquid decontaminant for solubilization of HD and especially thickened HD and GD. However, detoxification reactions are inhibited in low polarity solvents. Thus one must conduct a wide variety of optimization studies to arrive at a workable system.

Because of the chemical nature of HD, there can be no catalyst for substitution reactions such as hydrolysis. Catalysts for the substitution of VX are possible, but no effective catalyst has been found, perhaps because the leaving group in VX is so poor. The hydrolysis of G-agents can be effectively hydrolyzed by transition metal ions or by enzymes. The search now is for a catalyst which will operate in mildly acidic media where oxidative reagents for HD and VX will be more stable. Thereby one could have a system which would destroy G-agents by catalytic hydrolysis while another reagent, an oxidant, could take care of VX and HD.

A variety of enzymes have been found which will degrade the G-agents, however VX is only slowly degraded by enzymes such as parathion hydrolase. This enzyme needs to be improved, or new more effective enzymes must be discovered if we are to rely on enzymatic decontamination. HD cannot be destroyed enzymatically although its hydrolysis product thiodiglycol can be readily treated bacteriologically as shown by DeFrank at ERDEC. Characterization of the enzymes involved in this reaction could be a fruitful area of research.

Because of the low priority placed on decontamination research, there are many more high potential approaches to explore than there is funding to support. As long as funding levels remain low, successful identification of new decontamination systems will be delayed.



Department of Chemistry

111 Willard Hall
Manhattan, Kansas 66506-3701
913-532-6665
FAX: 913-532-6666

October 9, 1995

Dr. Reginald Seiders
Chemistry Division
U.S. Army Research Office
Attn: SLCRO-IP
P. O. Box 12211
Research Triangle Park, NC 27709-2211

Dear Reg,

Than you for arranging the recent workshop on Decontamination, Demilitarization. I found the topics covered and the presentations made to be very educational. The presence of DOD officials from all branches was also quite helpful.

Regarding suggestions I might make after hearing all the discussions.:

Wide-Area Decontamination

Suggestion:

- (1) Use enzyme plus NaOCl cocktails in a foaming type medium. The foam would cover the area and wet, immobilize, and destroy the agents. This assumes that hypochlorite and enzymes can be put in a compatible form.
- (2) Treat the area with MgO, Mg(OH)₂, CaO in high surface area form. They could also be the special [M_xO_y]CaO or MgO forms (M_xO_y = Fe₂O₃ or V₂O₅). Let us call these materials "super lime". Consider high surface CaO. This material is strongly basic, and when it hydrates to Ca(OH)₂, a great deal of heat is given off, and Ca(OH)₂ is also strongly basic. Slowly the excess Ca(OH)₂ will react with CO₂ and eventually become CaCO₃, a non-basic "rock". This dust could eventually be blown or washed away.

Note that MgO, Mg(OH)₂, CaO, Ca(OH)₂, and CaCO₃ are all nontoxic, but the oxides and hydroxides are quite reactive in high surface area forms. The materials are also fairly light, free flowing powders. High surface MgO or Mg(OH)₂ are particularly light.

Electronic Equipment

Suggestion:

- (1) Get approval to use the new refrigeration fluids as solvents. Incorporate collection and recycling as much as possible. Run the collected fluid-toxic agent mixture to an activated carbon to absorb toxic substance.

Decontaminating Large Equipment - Tanks, etc.

Suggestion:

- (1) Use DS2 or a new enzyme/hypochlorite cocktail.
- (2) Use a new polyoxometal ion/hypochlorite cocktail.
- (3) Dust thoroughly with "super-lime" as discussed under Wide Area Decontamination. Wash with water.



Individual Decon - Soldiers

Suggestion:

- (1) Use best activated carbon for rubbing on contaminated clothing, rifles, etc.
- (2) Perhaps a mixture of "super-lime" and activated carbon could be used so that some capability for destruction of the agents is also available.

(In general, the advantage of activated carbon is that it does not get wet and deactivated. However, it does not destroy the agent.

"Super-lime" should provide adsorbing and destruction capability. However, it would not be usable for gas masks nor could it be stored in open containers because over time it reacts with water and CO_2 .)

Of course, if a noncorrosive enzyme/ NaOCl cocktail can be developed, this could also be used by soldiers. But liquid based decon systems will be heavy to carry and somewhat corrosive.

Destruction of Stock Piled Agents

Toxic materials collected from the battlefield or collected from elsewhere could be destroyed using a heated cartridge filled with pellets of "super-lime." After use the cartridge could be treated with air at elevated temperatures, and then discarded as non-toxic.

Interior Decon

Suggestion:

- (1) Use new enzyme/hypochlorite cocktail
- (2) Use new polyoxometal ion/hypochlorite cocktail.

These are my suggestions after hearing all of the talks and discussions at the meeting. Perhaps I am overlooking something and the real chemical warfare experts would have to access how useful these suggestions are.

II. Future Workshops

Suggestions:

- (1) Dealing with Clean-up of Military Bases, Mixed Wastes, Contaminated Soils
- (2) Dealing with Military Radioactive Waste
- (3) Dealing with Contaminated Water Supplies

III. Needs of DOD

- * Alternative to incineration of toxics

* Ways of destroying chemical agents in air, eg. when a SCUD missile is hit by a Patriot Missile. (A crazy idea: Use Patriot Missiles carrying super-lime as part of the payload. A cloud of this material, which will probably be heated by the explosion may help destructively adsorb the chemical agent in the air.)

I hope these suggestions are of some use.

Yours truly,

Kenneth J. Klabunde
University Distinguished Professor

jh

Oklahoma State University

COLLEGE OF ARTS AND SCIENCES

Warren T. Ford, Regents Professor
E-mail: wtford@osuunx.ucc.okstate.edu

Department of Chemistry

107 Physical Sciences
Stillwater, Oklahoma 74078-0447
405-744-5920
FAX 405-744-6007
telephone 405-744-5946

9 October 1995

Dr. Reg Seiders
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

Dear Reg:

An abstract of my talk at the workshop is enclosed. This letter contains my comments and continuation of the Saturday morning discussion about the future of decon.

Decontamination problems are not solved. The question for DoD is the priority for R&D on decontamination of CBW. As threats to human life worldwide, they must be considered along with nuclear weapons in the hands of terrorist individuals and governments. They are poor men's nukes, and the most likely troublemakers are poor men. Similarly, investment in chemical and biological defense is cheap relative to nuclear defenses. Do we really need a renewed Star Wars program? For a tiny fraction of the cost, we could do so much more to counter the threat of chemical warfare.

Your discussion of decontamination challenges at the meeting was designed well to address unsolved problems. It avoided demilitarization, for which there are several good solutions that need to be evaluated, but do not require further basic research. I'll organize my comments to follow the discussion.

I. Wide Area Decontamination

A. Seaport and airports

These are Navy and Air Force needs. DS2 is unacceptable. The time scale of the operation must be hours, to get the facility back into use. New equipment, such as pumps, and new decontamination formulations are acceptable. The solution must be general for G agents, VX, and HD, and for thickened agents. Therefore, it must include organic solvent and/or a large amount of surfactant, which could be in the form of a microemulsion or micelles. Another essential component is excess base. Most of the discussions at the workshop ignored this point. **Hydrolysis of all of the agents requires 2 moles of base per mole of agent**, and to be sure of coverage, a huge excess of base must be applied in a real treatment. The preferred base may be calcium carbonate or calcium oxide, because they are insoluble and will leave only a powdered residue. The practical (slippery, corrosive surfaces) and environmental consequences of huge excesses of sodium hydroxide are unacceptable.

Sorbents are good for quick treatment, but in the long term must still be decontaminated. Therefore, they are probably unacceptable. How would a sorbent be collected for transport to a final decon facility?

Enzymes are likely too slow acting. Nobody at the workshop was able to address the problem of mass transport of agent to enzyme. How does one insure contact between a glob of thickened agent and the enzyme?

Latex dispersions or polyelectrolyte solutions might be applied as a catalyst-containing component of a mixture, but organic solvent or surfactant that dissolves mustard, VS, and thickeners will be essential. The solvent should evaporate within a few hours to make the site habitable.

B. Agricultural land

Here the time scale of the operation could be days or weeks. From an environmental standpoint, enzymes seem like better decontaminants than a slow-degrading organic chemical. Degradable surfactants would need to be cheap. With enzymes or chemicals, we probably don't need to be concerned with providing base, for the soil is a huge reservoir of buffer.

II. Sensitive equipment

Water is not allowed. Supercritical carbon dioxide seems like the most promising approach because it rinses agent out of the equipment. An absorbent would trap the agent, but still would have to be physically cleaned out. Would absorbent dispersed in supercritical carbon dioxide be an improvement? In any case, the solids left after venting of the carbon dioxide and sorbents loaded with agent still require decontamination, but that treatment can be done by a variety of methods specific to the agent at a later time.

III. Interiors of vehicles and buildings

Water may not be acceptable. Ozone or some other gas fumigant seems possible. Regardless of the decontamination material, later cleanup with detergent and water will be necessary to remove residues of agent byproducts. In this case, maybe a microemulsion, micellar, or latex spray, with organic solvent that evaporates, as in large area decon might even work.

IV. Individuals

This topic was not addressed thoroughly in the workshop discussion.

The absorbent XE-555 is a good first step for skin decon. It could be improved by inclusion of catalyst and stoichiometric base. Simply putting acidic and basic ion exchange resins into the formulation does not result in decontamination. Latex catalysts and calcium oxide or calcium carbonate might be used in the next generation. I understood from the discussion that 3 candidates to replace XE-555 are under evaluation, and that all are cheaper than XE-555. Basic alumina might be a good candidate from the standpoint of decontamination combined with sorbent properties.

Decontamination of the entire protective suit is needed to get the soldier back into action. An absorbent is not enough here. I assume that water would be the only liquid available in the field. It might be possible to transport dry surfactant, dry base such as calcium oxide, and dry latex and disperse them in water when needed. Dry mixtures of oxidants, bases, catalysts, and surfactants that can be dispersed in water and sprayed with minimal equipment, such as for small gardens, are likely solutions. The dry oxidant probably has to be a source of NaOCl.

Protection was not included in the discussion, but is an essential element of individual decontamination. Without it the individual is dead or in need of immediate medical attention. Latex catalysts and stoichiometric calcium oxide could be built into the fabric of the protective suit along with the active carbon now used. In principle, a polymeric catalyst could be used in the form of fibers, but I am not aware of fibers of a base such as calcium oxide.

V. Large equipment - tanks and trucks

This was not in your outline, but the discussion arose anyway. DS2 works and for economic reasons should not be trashed. It's like asbestos pipe insulation. The best thing to do is leave it in place until it becomes absolutely necessary to dispose of it.

Treatment to make material suitable for shipment back to the United States can be agent specific and has no urgent time limit, so all of the other possible solutions discussed above may be considered.

I will contact my US Representative and Senators about chemical defense matters. I assume that arguments for support of chemical defense within the DoD should be left to DoD personnel. Can you suggest any other approaches I could take to influence DoD priorities toward chemical defense problems in a time of limited resources?

Sincerely yours,

Warren

THE STATE UNIVERSITY OF NEW JERSEY
RUTGERS

Department of Chemistry • Wright-Rieman Laboratories • New Brunswick • 908/932-2618
Postal Address: P.O. Box 939 • Piscataway • New Jersey 08855-0939

October 9, 1995

Dr. Reginald Seiders
Chief, Organic Chemistry
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709

Dear Reg:

I am writing to express my thanks for your good work in organizing the Workshop on Decontamination. I learned a lot, and I was particularly impressed by the cross-fertilization that came from hearing about the many varied approaches that can be taken to the family of related decon problems. It was a most useful experience, one that should affect the way we all plan our research.

It would most certainly be useful to hold future workshops--perhaps at 2 year intervals. I don't think that this is redundant relative to the ERDEC November meetings. There, only 1 afternoon of Decon is scheduled. Here we had 5 concentrated sessions with a committed and focused audience. I really felt that I was both learning and helping to teach.

You may remember that I indicated that my abstract, brief though it was, was misprinted in the brochure (a line was omitted). I am enclosing a correct version for your report.

Once again, thanks for providing this excellent interface.

With best personal regards,

Sincerely,



Robert A. Moss
L.P. Hammett Professor

CONFERENCE ROSTER
ARMY RESEARCH OFFICE/DECONTAMINATION CONFERENCE
October 4- 7, 1995

JAMES BAKER
U.S. ARMY ERDEC
SCBRD RT
ABERDEEN PROVING MD 21010
410-671-4144

SALVATORE BOSCO
DEPARTMENT OF DEFENSE
3050 DEFENSE PENTAGON
OATSD (AE) (C/BM)
WASHINGTON DC 20301
703-602-5620

JOSEPH BUNNETT
UNIVERSITY OF CALIFORNIA
DEPARTMENT OF CHEMISTRY
SANTA CRUZ CA 95064
408-459-2261

JIK CHIN
MCGILL UNIVERSITY
DEPARTMENT OF CHEMISTRY
MONTREAL
CANADA H3A 2K6

DONALD CRONCE
NAVAL WARFARE CENTER
17320 DAHLGREN ROAD B51
DAHGREN VA 22448
540-653-8621

RUSSELL DRAGO
UNIVERSITY OF FLORIDA
2281 NW 24TH AVENUE
GAINESVILLE FL 32605
904-392-6737

HAL GUARD
OFFICE OF NAVAL RESEARCH CD 331
800 NORTH QUINCY STREET
ARLINGTON VA 22217
201-724-3016

CRAIG HILL
EMORY UNIVERSITY
DEPARTMENT OF CHEMISTRY
ATLANTA GA 30322
404-727-6611

FRED BERG
U.S. ARMY
703 FOX BOW DRIVE
BELLAIR MD 21014
410-671-2131

JOE BRUMFIELD
OFFICE OF NAVAL RESEARCH
800 NORTH QUINCY STREET
ARLINGTON VA 22217-5000
703-696-4319

CLIFFORD BUNTON
UNIVERSITY OF CALIFORNIA
DEPARTMENT OF CHEMISTRY
935 COCOPAH DRIVE
SANTA BARBARA CA 93110
805-893-2605

JOHN COOPER
LLNL
P. O. BOX 808, L-369
LIVERMORE CA 94551
510-423-9949

JOSEPH DE FRANK
U.S. ARMY ERDEC
SCBRD/RTL BUILDING E 3220
ABERDEEN PROVING MD 21010
410-671-3749

WARREN FORD
OKLAHOMA STATE UNIVERSITY
DEPARTMENT OF CHEMISTRY
STILLWATER OK 74078
405-744-5946

MILTON HARRIS
UNIVERSITY OF ALABAMA
DEPARTMENT OF CHEMISTRY
HUNTSVILLE AL 35899
205-895-6377

JOE HOVANEC
U.S. ARMY ERDEC
OFFICE CODE SCBRD RTC
ABERDEEN PROVING MD 21010
410-671-2761

ARMY RESEARCH OFFICE/DECONTAMINATION CONFERENCE

DAVID JAEGER
UNIVERSITY OF WYOMING
P. O. BOX 3838
LARAMIE WY 82070
307-766-4335

FREDRICK LONGO
SCITECH SERVICES, INC.
1232 PLAZA CIRCLE
JOPPA MD 21085
410-671-3719

KENNETH MCKENNA
DOD PROGRAMS OFFICE
LANL, MS-A133
LOS ALAMOS NM 87545
505-667-1992

GEORGE MERKEL
ARMY RESEARCH LAB
5412 INVERCHAPEL ROAD
SPRINGFIELD VA 22151
301-394-2290

BRIAN MacIVER
US ARMY ERDEC
SCIENCE & TECH SCBRD/RTC
ABERDEEN PROVING MD 21010
410-671-5919

DONALD PETTIT
LOS ALLAMOS NATIONAL LAB
D462
LOS ALAMOS NM 87545
505-667-6843

FRANK RAUSHEL
TEXAS A & M UNIVERSITY
DEPARTMENT OF CHEMISTRY
COLLEGE STATION TX 77843
409-845-3373

ALAN RUSSELL
UNIVERSITY OF PITTSBURGH
CHEMICAL ENGINEERING
1249 BENEDUM HALL
PITTSBURGH PA 15261
412-624-9631

KENNETH KLABUNDE
KANSAS STATE UNIVERSITY
DEPARTMENT OF CHEMISTRY
MANHATTAN KS 66056
913-532-6849

RAY MCKAY
CENTER FOR ADVANCED MATERIALS
BOX 5665
POTSDAM NY 13699
315-268-2336

FRED MENDER
EMORY UNIVERSITY
DEPARTMENT OF CHEMISTRY
ATLANTA GA 30222
404-727-6599

ROBERT MOSS
RUTGERS UNIVERSITY
DEPARTMENT OF CHEMISTRY
NEW BRUNSWICK NJ 08903
908-445-2606

GEORGE NEWKOME
UNIVERSITY OF SOUTH FLORIDA
4202 EAST FOWLER AVENUE ADM200
TAMPA FL 33620
813-974-5481

LARRY PROCELL
ERDEC/ RESEARCH & TECHNOLOGY
BUILDING E3300 APG EA
ABERDEEN PROVING MD 21010
410-671-8475

ROY ROTH
U.S. ARMY RESEARCH
P. O. BOX 12211
RESEARCH TRIANGLE NC 27709
919-549-4346

REG SEIDERS
ARMY RESEARCH OFFICE
P. O. BOX 12211
RESEARCH TRIANGLE NC 27709-2211
919-549-4365

ARMY RESEARCH OFFICE/DECONTAMINATION CONFERENCE

GARY SELWIN
LOS ALAMOS NATIONAL LABORATORY
MAIL STOP E 526
P. O. BOX 1663
LOS ALAMOS NM 87545
505-665-7359

SANDRA SHURMAN
U.S. AIR FORCE
8107 13TH STREET
BROOKS AFB TX 78235
210-536-4533

CRAIG TAYLOR
LOS ALAMOS NATIONAL LAB
MAILSTOP G-740
LOS ALAMOS NM 87545
505-667-7236

GEORGE WAGNER
GO CENTERS INC.
GUN POWDER BRANCH
P. O. BOX 68
ABERDEEN PROVING MD 21010
410-671-8468

KEITH WARD
NAVAL RESEARCH LABORATORY CD6030
4555 OVERLOOK AVENUE SW
WASHINGTON DC 20375
202-767-2735

ANNETTA WATSON
OAK RIDGE LAB/HEALTH SCIENCE
BUILDING 4500 SOUTH
MAIL STOP 6101/P. O. BOX 2008
OAK RIDGE TN 37831
615-562-125

JOHN WEIMASTER
ERDEC RESEARCH & TECH
SCBRD RTC
ABERDEEN PROVING MD 21010
410-671-4148

NGAI WONG
AIR FORCE ARMSTRONG LABS
US ARMY CBD COM
AMSCB-AL BUILDING E #32-34 APG
ABERDEEN PROVING MD 21010
410-671-3111

YU-CHU YANG
EDGEWOOD RESEARCH DEVELOPMENT
ENGINEERING CENTER ERDEC
U.S. ARMY
ABERDEEN PROVING MD 21010
410-671-8483

TOTAL NAMES LISTED= 41

New Concepts in Decontamination Workshop

Overall Workshop Evaluation

| | Satisfied | | 3 | 4 | Dissatisfied | |
|--|-----------|----|---|---|--------------|-----|
| | 1 | 2 | | | 5 | N/A |
| 1. Preworkshop Publicity & Information | 8 | 3 | 4 | 2 | 1 | 1 |
| 2. Preregistration | 10 | 4 | 2 | | | |
| 3. On-site registration | 14 | 2 | | | | |
| 4. Lodging Rooms | 11 | 4 | 1 | | | |
| 5. Breakfasts, breaks | 9 | 6 | 1 | | | |
| 6. Meeting Facilities | 9 | 6 | 2 | | | |
| 7. Length of Workshop | 11 | 6 | | | | |
| 8. Amount of Free Time | 10 | 6 | 1 | | | |
| 9. Date of Workshop | 9 | 6 | | 2 | | |
| 10. Location of Workshop | 16 | 1 | | | | |
| | Yes | No | | | | |
| 11. Did you know what the goals and objectives of the workshop were? | 15 | 1 | ? | | | |
| 12. In your opinion, were they met? | 13 | 1 | ? | | | |
| 13. Would you recommend this workshop to a friend or associate? | 16 | 1 | | | | |